SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED	1b. RESTRICTIVE MARKINGS N/A
2a. SECURITY CLASSIFICATION AUTHORITY AD-A281 367	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited
S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION Cornell University	6b. OFFICE SYMBOL (If applicable)
6c. ADDRESS (City, State, and ZIP Code) Office of Sponsored Programs 123 Day Hall Ithaca, NY 14853	7a. NAME OF MONITORING ORGANIZATION 7b. ADDRESS (City, State, and ZIP C
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Office of Naval Research	8b. OFFICE SYMBOL (If applicable) ONR
8c. ADDRESS (City, State, and ZIP Code) 800 N. Quincy St., 614A:DHP Arlington, VA 22217-5000	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N00014-90-J-1948
	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. / PROJECT NO. / TASK NO. / WORK UNIT ACCESSION NO.

DTIC ELECTE JUL 08 1994 S G D

11. TITLE (Include Security Classification)
UNCLASSIFIED: Carbon Clusters Studied by Neutralization-Reionization Mass Spectrometry

12. PERSONAL AUTHOR(S)
Fred W. McLafferty

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final Report	FROM 1991 TO 1994	94/06/25	3

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Neutralization-Reionization Mass Spectrometry Neutral Carbon Clusters

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

DTIC QUALITY INSPECTED 5

Ab initio calculations of isomeric carbon clusters C_n^0 and C_n^+, n = 2-4, yield structures and energies similar to previous reports, although five (not two) C_4^+ structures have local energy minima. Dissociative ionization of structurally varied precursors was used to prepare C_3 and C_4 ionic and neutral isomers; however, their mass spectra from collisionally activated dissociation (CAD) and neutralization-reionization (NR) under a wide variety of conditions are indistinguishable, indicating only one isomer or the same mixture of isomers. Likewise, CAD and NR spectra of C_4^+ and C_4^0 from $^{13}CH_2{=}CHCH{=}^{13}CH_2$ and C_3^+ and C_3^0 from $CH_2{=}^{13}CHCH_3$ show complete $^{13}C/^{12}C$ scrambling. CAD cross sections are consistent with C_4^+ - C_6^+ ions as mainly linear isomers and C_7^+ ions from cyclic precursors as mainly cyclic. Product abundances from the unimolecular dissociation of C_n^0, C_n^-, and C_n^+ allow the selection of thermodynamic data that should be of higher relative accuracy, such as 11.4 eV for the C_3 ionization energy from reported values of 10.0-13.0 eV.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION	
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	UNCLASSIFIED	
22a. NAME OF RESPONSIBLE INDIVIDUAL Fred W. McLafferty	22b. TELEPHONE (Include Area Code) 607/255-4699	22c. OFFICE SYMBOL

DD Form 1473, JUN 86 — Previous editions are obsolete. — SECURITY CLASSIFICATION OF THIS PAGE

OFFICE OF NAVAL RESEARCH

FINAL REPORT

for

GRANT: N00014-90-J-1948

R&T Code 1113/91/RAD

Carbon Clusters Studied by Neutralization-Reionization Mass Spectrometry

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Date Submitted: June 9, 1994

SMALL CARBON CLUSTERS (C_n^0, C_n^+, C_n^-) FROM ACYCLIC AND CYCLIC PRECURSORS. NEUTRALIZATION-REIONIZATION MASS SPECTROMETRY AND THEORY

The chemistry of C_n molecules and ions in plasmas (carbon arcs, laser ablation) and in the formation of polynuclear aromatics, diamond films, and soot has been the subject of extensive theoretical and experimental research. In these studies, ab initio calculations of isomeric carbon clusters C_n^0 and C_n^+, n = 2-4, yield structures and energies similar to previous reports, although five (not two) C_4^+ structures have local energy minima. Dissociative ionization of structurally varied precursors was used to prepare C_3 and C_4 ionic and neutral isomers; however, their mass spectra from collisionally activated dissociation (CAD) and neutralization-reionization (NR) under a wide variety of conditions are indistinguishable, indicating only one isomer or the same mixture of isomers. Likewise, CAD and NR spectra of C_4^+ and C_4^0 from $^{13}CH_2{=}CHCH{=}^{13}CH_2$ and C_3^+ and C_3^0 from $CH_2{=}^{13}CHCH_3$ show complete $^{13}C/^{12}C$ scrambling. CAD cross sections are consistent with C_4^+ - C_6^+ ions as mainly linear isomers and C_7^+ ions from cyclic precursors as mainly cyclic. Product abundances from the unimolecular dissociation of C_n^0, C_n^-, and C_n^+ allow the selection of thermodynamic data that should be of higher relative accuracy, such as 11.4 eV for the C_3 ionization energy from reported values of 10.0-13.0 eV.

Technical Reports and Journal Articles:

362. McLafferty, F.W. Neutralization-Reionization Mass Spectrometry, Int. J. Mass Spectrom. Ion Processes **1992**, 118/119, 221-235.

377. Fura, A.; Turecek, F.; McLafferty, F.W. Small Carbon-Clusters (C_n^0, C_n^+, C_n^-) from Acyclic and Cyclic Precursors. Neutralization-Reionization Mass Spectrometry and Theory, J. Am. Chem. Soc., submitted.

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Fred W. McLafferty, Principal Investigator, Professor of Chemistry

OFFICE OF NAVAL RESEARCH
PUBLICATIONS/PATENTS/PRESENTATIONS/HONORS REPORT

R&T Number: 1113/91/RAD
Contract/Grant Number: N00014-90-J-1948
Contract/Grant Title: Carbon Clusters Studied by Neutralization-Reionization Mass Spectrometry
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a. Number of papers submitted to refereed journals, but not published: 2
b. Number of papers published in refereed journals (list attached)*: 0
c. Number of books or chapters submitted, but not yet published: 0
d. Number of books or chapters published (list attached)*: 0
e. Number of printed technical reports & non-refereed papers (list attached)*: 0
f. Number of patents filed: 0
g. Number of patents granted (list attached)*: 0
h. Number of invited presentations at workshops or professional society meetings: 1
i. Number of presentations at workshops or professional society meetings: 2
j. Honors/Awards/Prizes for contract/grant employees (list attached)*: 0
(This might include Scientific Society Awards/Offices, Promotions, Faculty Awards/Offices)
k. Total number of Graduate Students and Post-Doctoral associates supported by at least 25% during this period, under this R&T project number:
Graduate Students: 2
Post-Doctoral Associates: 1
including the number of,
Female Graduate Students: 0
Female Post-Doctoral Associates: 0
the number of
Minority* Graduate Students: 1
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Enclosure (1)